Towards a systematic

statistical evaluation of diverse plankton-/ecosystem models

against data from

mesocosm experiments

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Bundesministerium
für Bildung
und Forschung

Motivation

Description of the session A3: "… .The session will… bring together… the modelling and the observational community. It can thus be used as… a base for the exchange of information… ."

Added value & confidence in model results

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Added value: Numerical models provide and test information of process interactions that are difficult to measure directly, if at all.

Added value & confidence in model results

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Questions with respect to added value:

- Simulation results → confidence?
- Process assumptions → more confidence?
- Model selection → gained confidence yes/no?

Statistical (data-based) analysis of marine ecosystem models

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Answers require statistical, data-based model analyses of:

- parameter values (constant rate estimates)
- data-model misfits (systematic errors)
- structural model complexity (model redundancy)
- model sensitivities (degree of freedom)

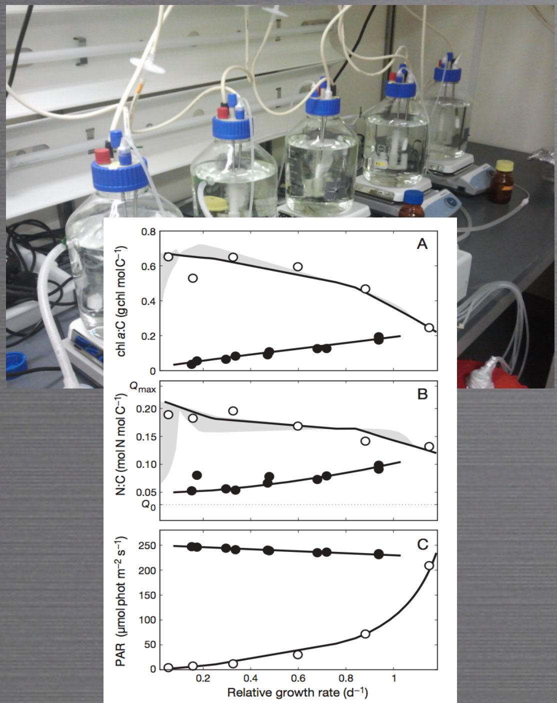
→ ***thousands of model runs!***

Model evaluation/assessment & computational time

Model evaluation against laboratory data

Computational time (one model run): **seconds – minutes**

- selected species (batch cultures)
- balanced growth conditions (chemostats)
- controlled environmental conditions



Wirtz & Pahlow (2010)

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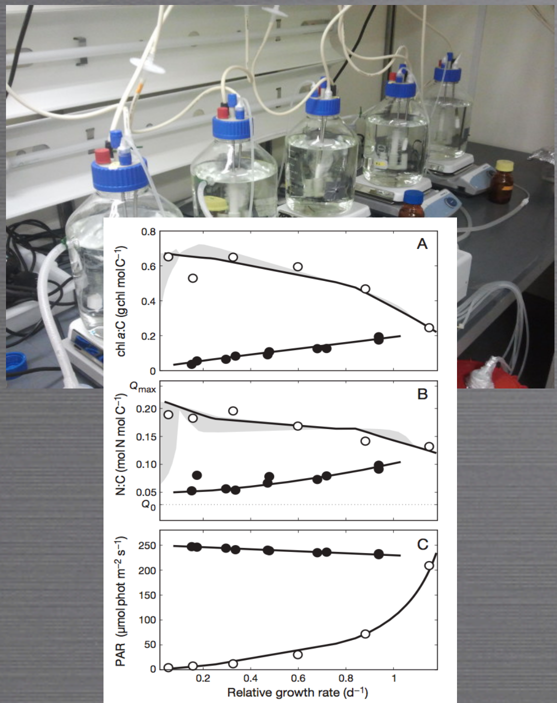
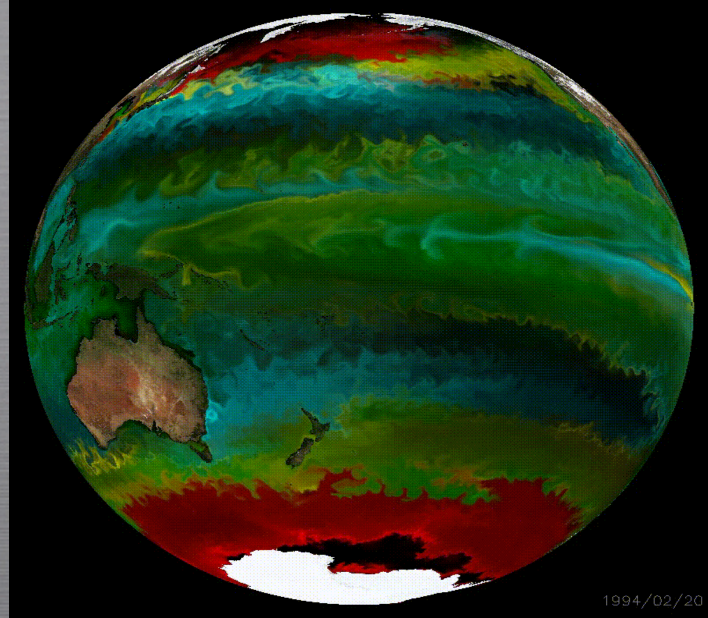


Wirtz & Pahlow (2010)

Prior information →

Simulation of dominant plankton species distribution Mick Follows et al. 'the darwin project' (media library, MIT)



Model evaluation against ocean data (global scale)

Computational time (one model run): **hours – months**

- myriad of species
- mainly transient growth conditions
- continuously varying environmental conditions

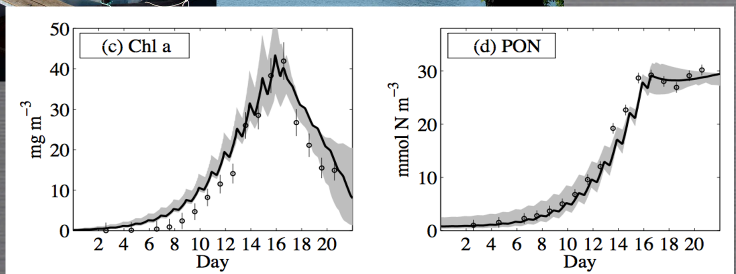
Model evaluation/assessment & computational time

Model evaluation against mesocosm data

Computational time (one model run): **seconds – minutes**

- various species (local natural plankton community)
- mainly transient growth conditions
- varying but measured environmental conditions

http://peece.ifm-geomar.de/images/Comparison)



Schartau et al. (2007)

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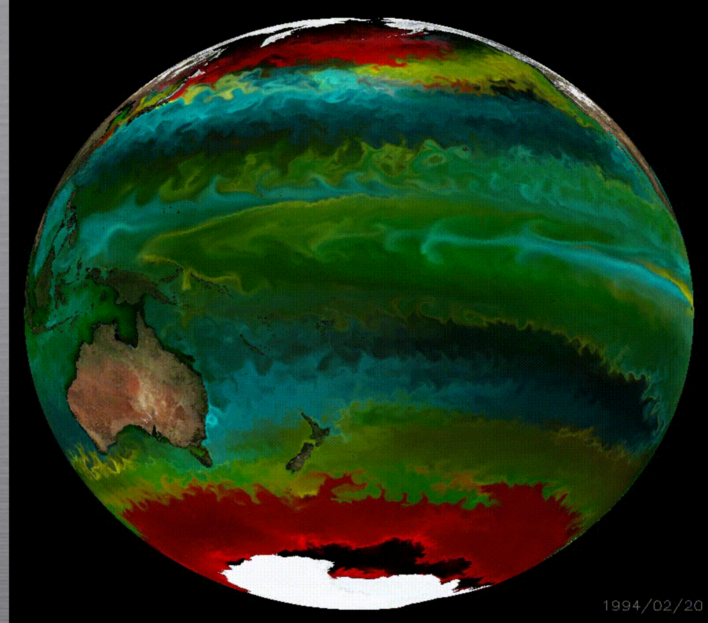

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Model evaluation/assessment & computational time

Usage of mesocosm data

http://peece.ifm-geomar.de/images/

Model evaluation,
parameter optimization,
sensitivity analysis,
cross-validation
→ thousands of model runs: **hours – days**

Prior information about model uncertainties:
confidence limits of parameter estimates & model results

Approaches in marine ecosystem modelling

Which model approaches are currently applied?

- Nutrient, phytoplankton, zooplankton, detritus (NPZD)
- Plankton functional type (PFT) models
- Size-based models
- Adaptive or optimality, trait-based models
- Carbon, nitrogen, phosphorus (CNP-) regulated models

etc.

Model 1, NPZD

Model 2, PFT

Model 3, trait-based

Model #N, …

Data series of mesocosm experiments

Which data are (or will become) **available?**

- PeECE I-III (Pelagic Ecosystem CO_2-Enrichment Studies) (e.g. Riebesell et al., 2008, BG)
- Boknis Eck experiment 2009 with Kiel Off-Shore Mesocosms for Future Ocean Simulations (KOSMOS) (e.g. Engel et al., 2014, JPR)
- Svalbard (Arctic) experiment 2010 (e.g. Schulz et al., 2013, special issue BG)
- Bergen experiment 2011 with KOSMOS (e.g. Endres et al., 2014, PlosOne)
- Tvärminne (Baltic Sea) experiment (2012)
- Kristineberg (Gullmar Fjord) long-term experiment (2013)

Exp 1, PeECE I

Exp 3, PeECE III

Exp 5, Svalbard

Exp #N, …

Workbench for model evaluation – simulations of mesocosom experiments

in Excel &/or NetCDF

- Exp 1, PeECE I
- Exp 3, PeECE III
- Exp 5, Svalbard
- Exp #N, …

in FORTRAN

- Model 1, NPZD
- Model 2, PFT
- Model 3, trait-based
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Workbench for model evaluation – simulations of mesocosom experiments

Environmental conditions: mesocosm specific files
Model parameter values: model specific namelist files
Iinitial conditions: model & mesocosm specific files

E#1M1
M#id1_param
E#2M#5_ini

in Excel &/or NetCDF

Exp 1, PeECE I
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Exp #N, …

Specification:
1) model
2) experiment & mesocosm
3) model parameter values

in FORTRAN

Model 1, NPZD
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R package FME
(Soetaert and Petzoldt, 2010,
Journal of Statistical Software)

in FORTRAN

Model 1, NPZD
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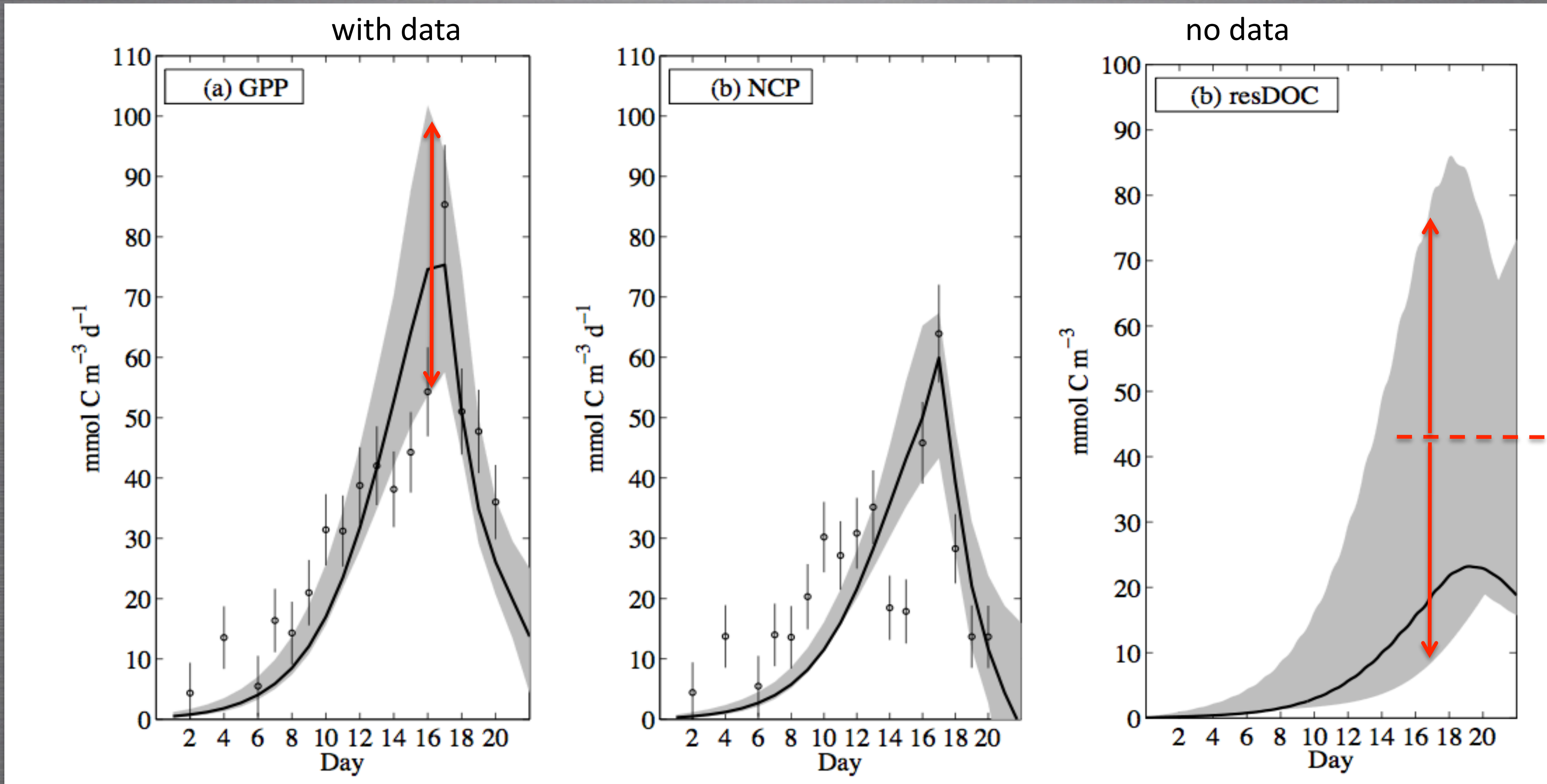
Model #N, …

Example of data-model analysis: uncertainty and data constraints

Good agreement: Gross primary production (GPP), net community production (NCP)
Badly constrained*: residual/fresh* dissolved organic carbon (resDOC)

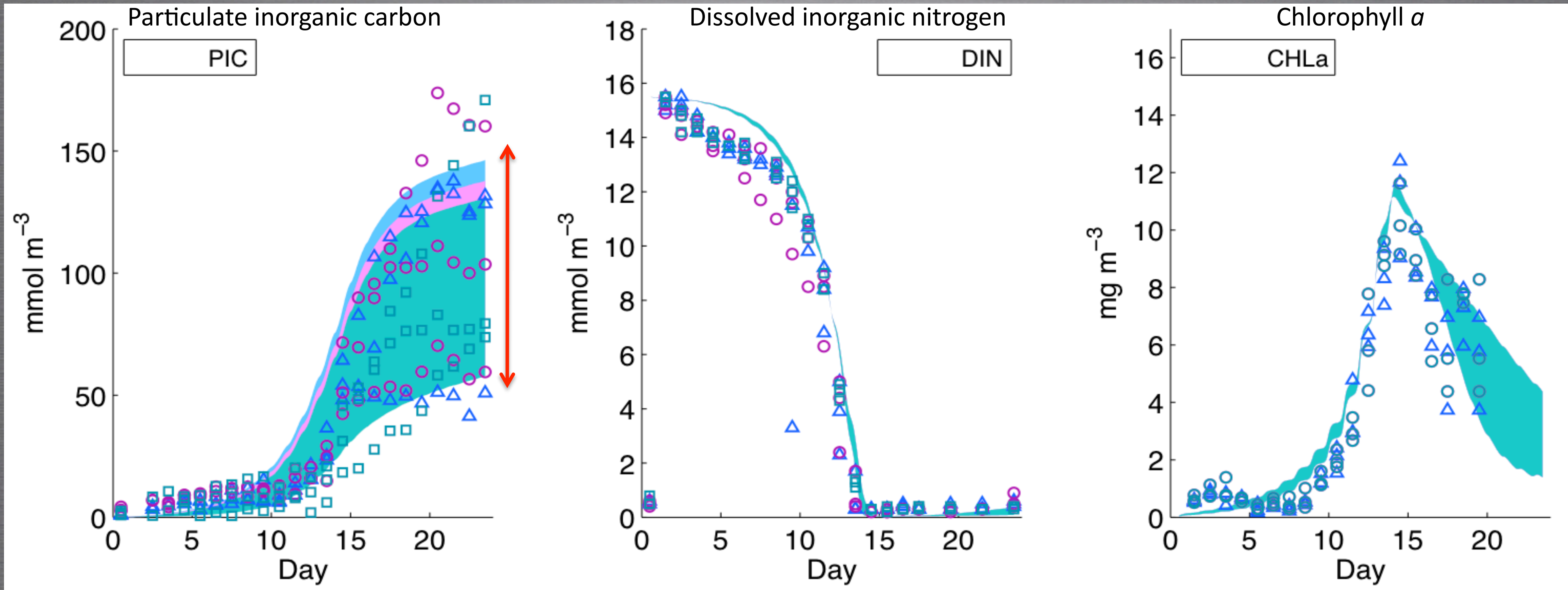


Modified from Schartau et al. (2007), Biogeosciences

Example of data-model analysis: variability and CO_2/pH response signal

$pCO_2 \approx 200\ ppm_v$
$pCO_2 \approx 400\ ppm_v$
$pCO_2 \approx 700\ ppm_v$

Observed and simulated variability



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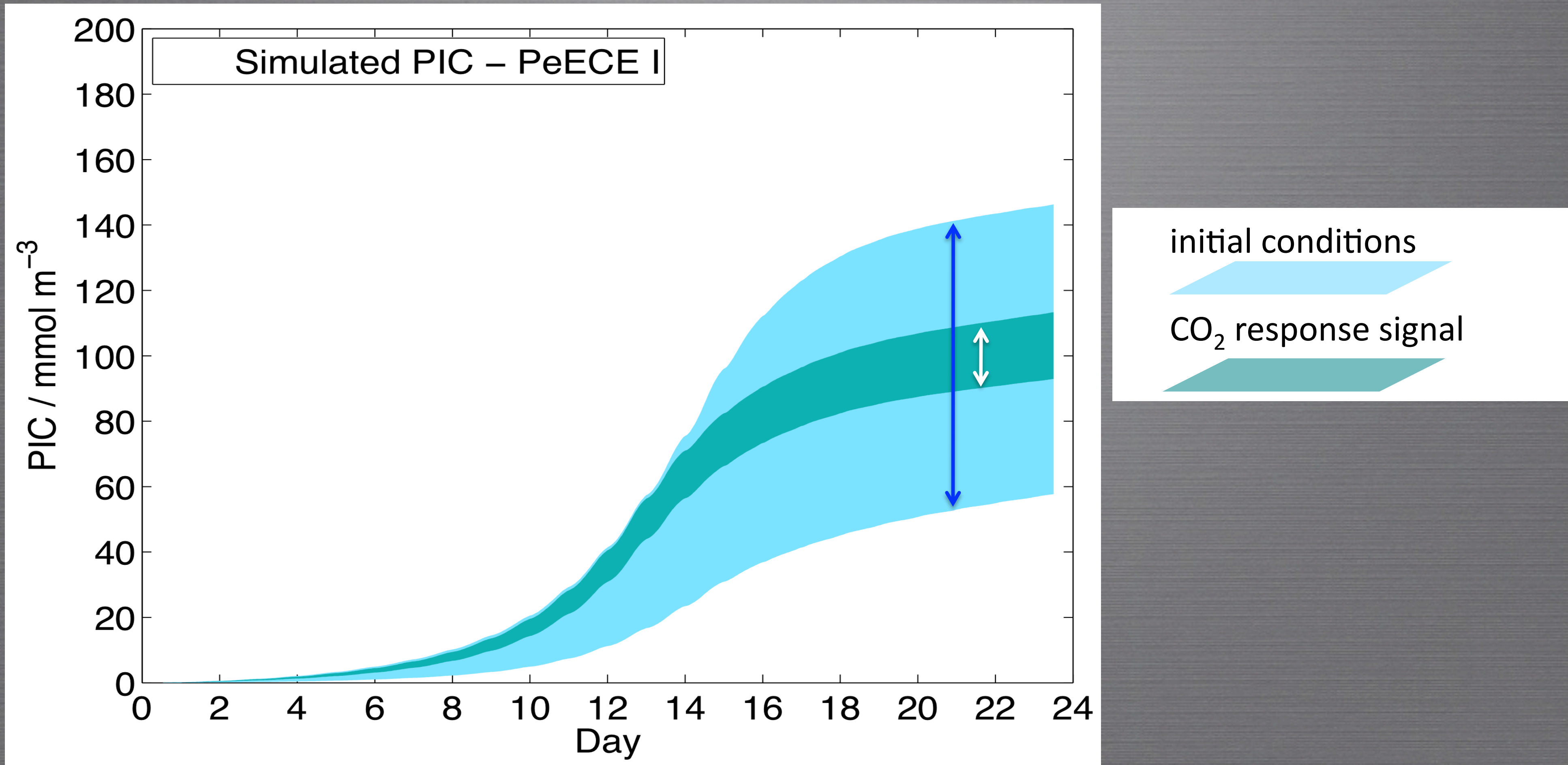
Example of data-model analysis: variability and CO_2/pH response signal

Observed and simulated variations in particulate inorganic carbon (PIC)

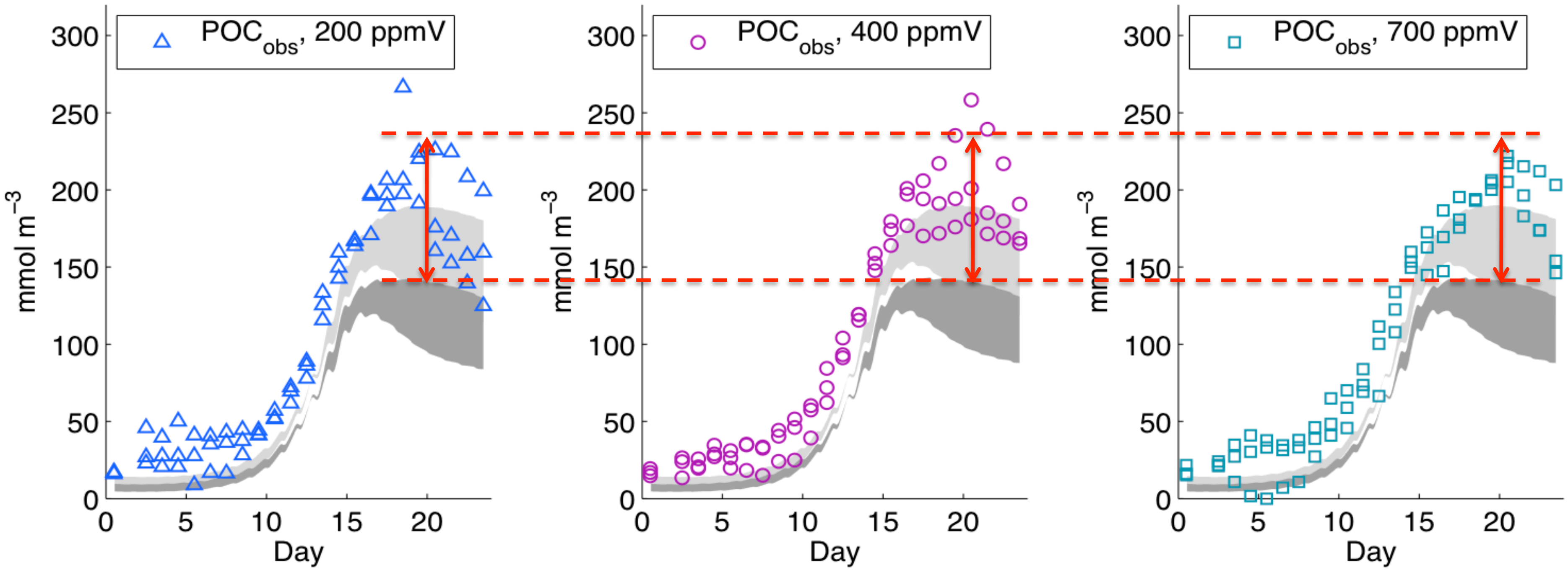


Example of data-model analysis: systematic data-model misfit

What is the correct model counterpart to measurements of particulate organic carbon (POC)?

simulated POC = PHY-C + HET-C + DET-C?

simulated POC = PHY-C + HET-C + DET-C
+ gel particles?



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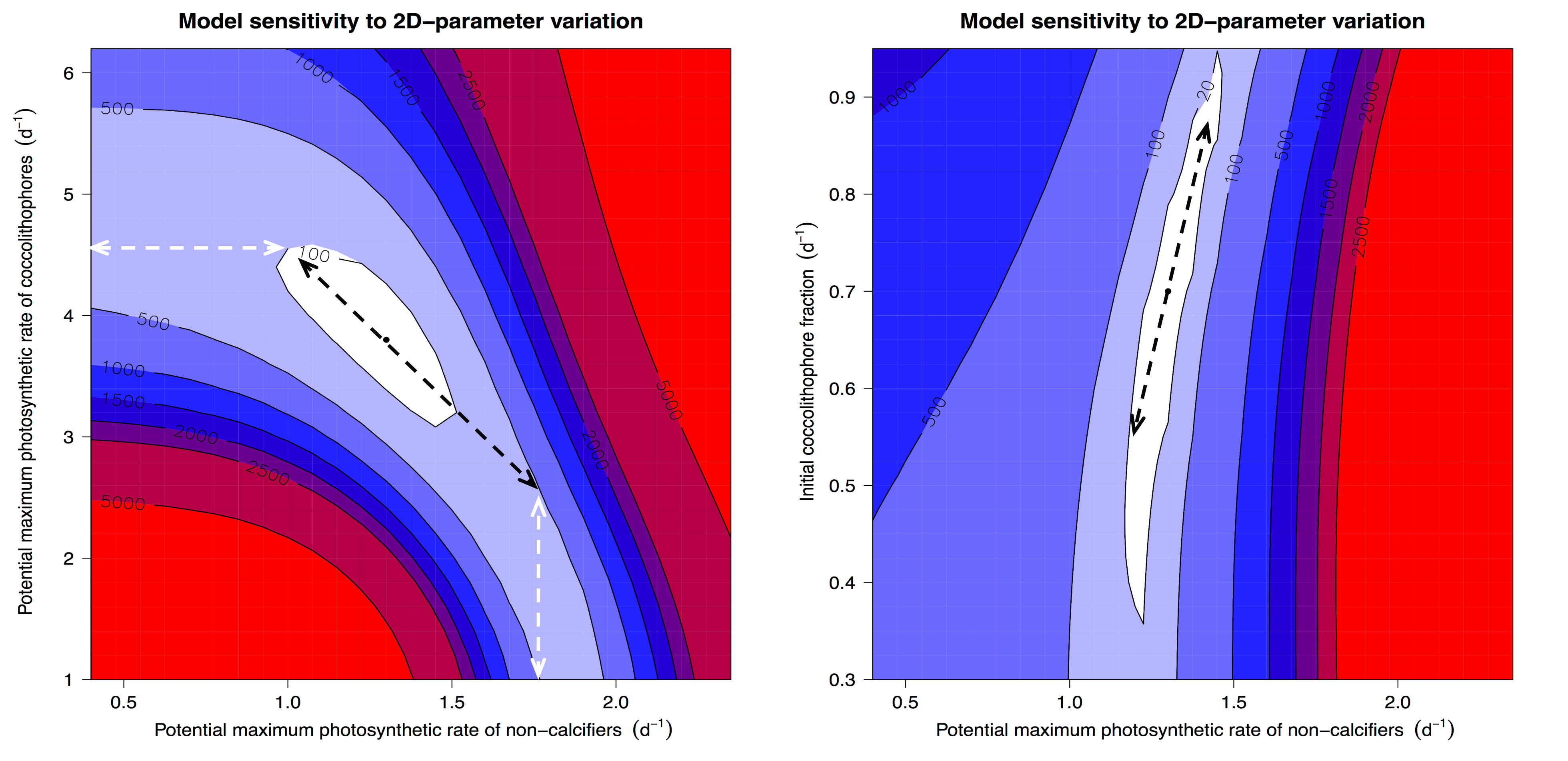
Example of data-model analysis: parameter correlations & confidence limits

Identical twin experiments (model deviation from reference solution at dates of observation)
→ changes in misfit (cost) function due to 2D-variations of parameter values



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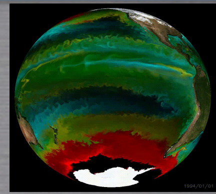
Summary & outlook

Prior information

Prior



(M. Follows and colleagues, media library, MIT)

Summary:

- to bring together the modelling and the observational community requires a good communication of the added value of model solutions (benefits and limitations)

- the added value of models can be substantiated with statistical evaluations of model performance, (which is a matter of computational time and data availability)

- statistical model evaluations are feasible & meaningful with data from mesocosm experiments

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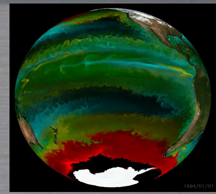

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Outlook:

- expansion of working environment → more mesocosm experiments and additional models

- extend compatibility → driver for Framework for Aquatic Biogeochemical Models (FABM)

  Bruggeman & Bolding, 2014

- find partners!(?) →

arcplan.com

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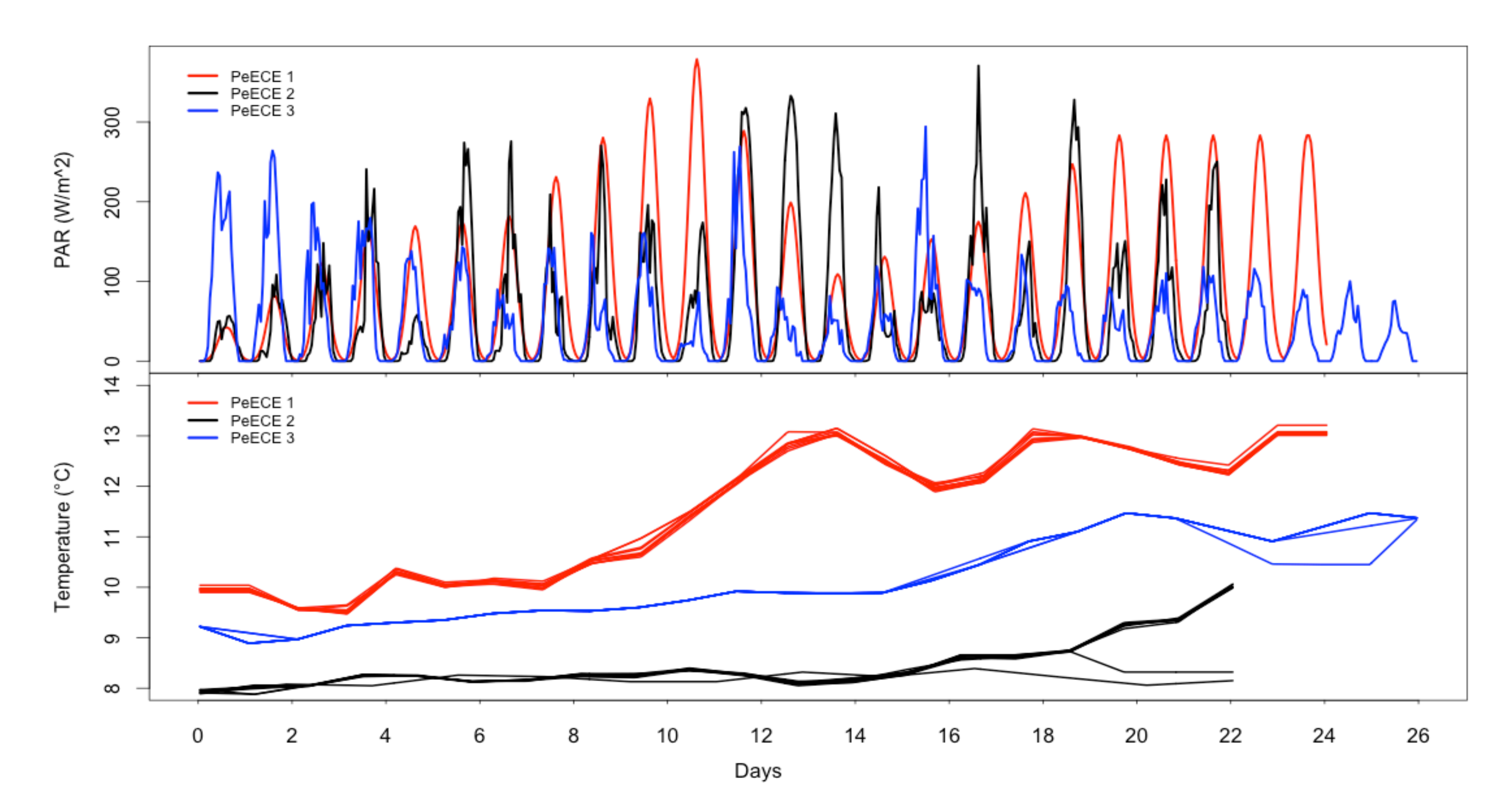
Experiment and mesocosm specific files: T, S, PAR, pCO_2atm

Temperature (T), Salinity (S), Photosynthetic available radiation (PAR), atmospheric CO2 (pCO_2atm)
Example: PAR and T (hourly values)



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PeECE – I data and test runs with refined CN-REcoM (Schartau et al., 2007)